DOCTORAL THESIS

THESIS BOOKLET

Analysis and control of nonlinear dynamic systems using novel computational methods

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2025

1 Introduction

Dynamic systems are widely used to describe a broad range of natural phenomena, including physical, mechanical, biological, chemical, and even sociological processes. Thus, an abstract, generic field of science with strong mathematical foundations and extensive literature has been developed for the analysis, synthesis, monitoring, and control of these models. The area still offers open questions: most theoretical results are only applicable for a well-defined subclass of the nonlinear systems, with a mathematical structure often too complex for an analytic solution. However, the emergence of modern computational hardware and methodologies opens the gate for solving previously non-tractable numerical problems in an acceptable time-frame. This thesis explores novel applications of computational methods, aimed at the observation, control, and parameter synthesis of nonnegative systems, with special focus on the compartmental epidemic models gaining unforeseen significance during the recent COVID-19 pandemic.

It is common in epidemiology to use different models for the evaluation of disease control strategies. Population-level deterministic epidemic models are most often written in a nonnegative compartmental form with polynomial nonlinearities representing the infection mechanism. Represented in the form of an ordinary differential equation (ODE) system, these are usually derived from a susceptible–(exposed)–infected–recovered (SEIR)-type description [1]. The nonlinearity makes the corresponding control problems challenging due to complex dynamical behavior, possible singularities, and the state-dependent nature of fundamental properties like reachability or observability [2].

COVID-19 was unprecedented in the sense that governments were forced to constantly tune their responses to find balance between public health concerns and the costs of social distancing measures to the society and the economy [3]. Formalisms like temporal logic can be an efficient choice for specifying such complex, time-varying conditions [4], with the possibility of algorithmic translation into a system of inequalities [5]. Model-predictive control is a straightforward approach to compute an optimal solution for nonlinear systems, taking into consideration complex goals and such constraints [6]. It can also incorporate additional inputs, like vaccination or testing intensity, which can significantly reduce the required stringency of social-distancing-type measures [7].

Most control algorithms require accurate and full state information of the target system, which is unrealistic to assume in the case of epidemic management (e.g. number of latent or asymptomatic infections). Both statistical methods and model-based solutions exist for the estimation of these values [8]. One possible approach is transforming the problem of data reconstruction into a control problem, where the model's output is used to track a reliably measurable quantity (like the number of hospitalizations). Stochastic MPC or a robust control method, together with a state observer, are among the possible choices.

Another important subset of nonnegative systems is the class of kinetic models, the dynamics of which can be formally represented by chemical reactions, assuming certain reaction rates. Due to the well-founded mathematical background [9], it is often beneficial to apply this framework even to originally non-chemical, but transformable models. Synthesizing parameters for such models, which guarantee a predefined qualitative behavior (e.g. a sustained chemical oscillation), has wide application possibilities. Not surprisingly, achieving this via traditional methods is challenging [10], but optimization-based approaches sometimes can provide an acceptable solution.

2 Basic notions and methodological background

2.1 Compartmental epidemic models

Compartmental epidemic models divide the population into disjunct groups (compartments), depending on the role they play in the transmission of the pathogen. In our work, we used different versions of the 8-compartment COVID-19 model, seen in Figure 1. Being a more complex version of the widely-known SIR (or SEIR)-type models, it has compartments for **S**usceptibles, **L**atently infected, **P**resymptomatic (already spreading the virus, but without symptoms yet), symptomatic **I**nfected, **A**symptomatic infected, **H**ospitalized, **R**ecovered, and **D**eceased.

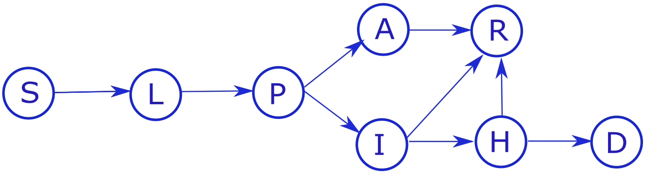


Figure 1: Transition diagram of an advanced nonlinear epidemic model

An important, widely applied metric for comparing the transmission speed of a pathogen, and consequently the stringency of (proposed) interventions in the case of COVID-19, is the time-dependent reproduction number. This shows the average number of individuals that a carrier will infect at a given time instance, and can be calculated for the base model as:

$$R_c(t) = \beta\,(1-u(t))\,\frac{S(t)}{N}\left(\frac{1}{p}+\frac{q}{\rho_I}+\frac{\delta(1-q)}{\rho_A}\right), \tag{1}$$

where $\beta, p, \rho_I, \rho_A, q, \delta$ are parameters related to the transmission rate, transmission probabilities, and relative infectiousness of compartments.

2.2 Model predictive control

Model predictive control (MPC) assumes a discrete dynamic model:

$$x_{k+1} = F(x_k, u_k). \tag{2}$$

At time instance k, the method expresses the future states for a finite, M-step horizon, noted $\mathbf{x}_k = \{x_{k+1|k}, \ldots, x_{k+M|k}\}$ as a function of the (yet unknown) future inputs $\mathbf{u}_k = \{u_{k|k}, \ldots, u_{k+M-1|k}\}$. It aims to find optimal control actions by minimizing a cost function of these future state and input values $J(\mathbf{u}_k, \mathbf{x}_k)$, solving the constrained optimization problem:

$$\min_{\mathbf{u}_k} J(\mathbf{u}_k, \mathbf{x}_k) \tag{3a}$$

$$\text{w.r.t.} \quad x_{k+i+1|k} = F(x_{k+i|k}, u_{k+i|k}) \tag{3b}$$

$$G_x(\mathbf{x}_k) \leq h_x, \; G_u(\mathbf{u}_k) \leq h_u \tag{3c}$$

Here, (3b) ensures the model-based dynamic behavior, and (3c) contains any additional user-defined constraints for the state and input values. Typically, a feedback is applied, periodically re-solving the problem in a shrinking-horizon (fixed end) or rolling-horizon fashion.

2.3 Feedback-linearization

Feedback-linearization is a technique for the linearization of a nonlinear input-affine system by applying a state-dependent nonlinear feedback. In the simplest case, starting from the continuous model:

$$\dot{x} = f(x) + g(x)\,u \tag{4a}$$

$$y = h(x), \tag{4b}$$

with f, g continuously differentiable as many times as needed, a state transformation can be defined using the derivatives of y (expressed using the Lie-derivatives of f, g and the relative degree ρ). By applying an input mapping in the form of $u = a(x) + b(x)v$, the transformed system:

$$z = \Phi(x) = \left(y, \dot{y}, \ldots, y^{(\rho-1)}\right)^T = \left(h(x), L_f h(x), \ldots, L_f^{\rho-1} h(x)\right)^T \tag{5}$$

will act as a linear system $\dot{z} = Az + Bv$ between the new input v and its output $y = z_1$. More precisely, it will behave as a simple cascade of integrators, for which any linear control technique (e.g. pole placement, LQR) can be applied to achieve a desired behavior (stability, asymptotic output tracking, etc). As presented in [2, Chap 4.3], $a(x), b(x)$ can be expressed as rational functions of the aforementioned Lie-derivatives.

3 Summary of the main results

3.1 Optimization-based epidemic control

The first step of optimization-based control is the specification of a cost function, a metric for quantifying the goodness of the obtained input and system behavior. The weight of different factors (e.g. economic damage, number of deaths, etc) in this cost will determine the nature of the optimal intervention strategy computed with MPC. Epidemic management strategies generally differentiate between the **suppression** of the epidemic (i.e., applying strict inputs/interventions to force the reproduction rate below 1 and eradicate the disease) or **mitigation** (where the aim is only keeping the number of simultaneous infections below a tolerable level, e.g. the capacity of healthcare resources).

As an example, Figure 2. presents the inputs obtained with a cost function mostly penalizing the economical damage, with a strict limit (10.000 people) on the hospitalization compartment. As temporarily releasable capacity, an additional 5.000 hospital places are allowed for the controller for a maximum of three weeks, whenever it finds it most beneficial. Due to practical constraints, changing the intensity of interventions is allowed only once every week. The resulting input corresponds to an optimal mitigation strategy, where - as observable around the end of the control horizon - lifting the restrictions results in the emergence of a new epidemic wave.

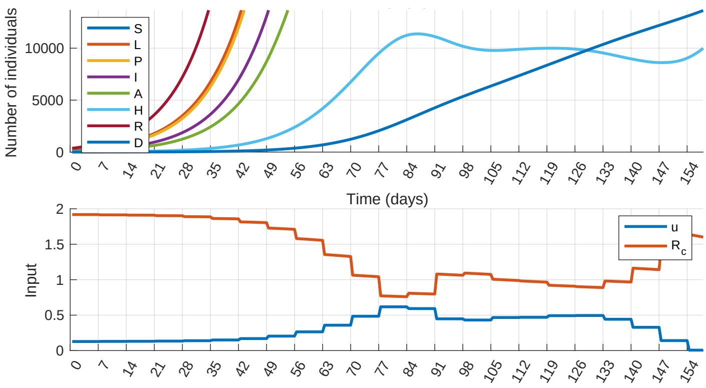


Figure 2: Simulated trajectories (top) and control inputs (bottom), optimizing for minimal economic damages while respecting a temporarily extendable healthcare capacity.

The required stringency of social distancing measures can be greatly reduced if additional inputs like vaccination and symptom-based testing are available. Figure 3. shows a case study comparing the required input stringency (v) and optimal schedule for the consumption of the limited number of tests available (κ) in case of vaccines with different efficiency (the different colors). Slightly different results can be observed if the number of tests usable in the given timeframe is also capped (dotted lines).

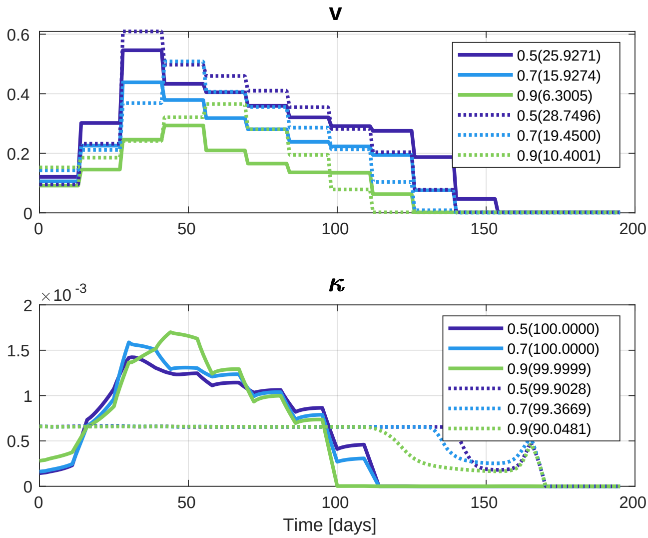
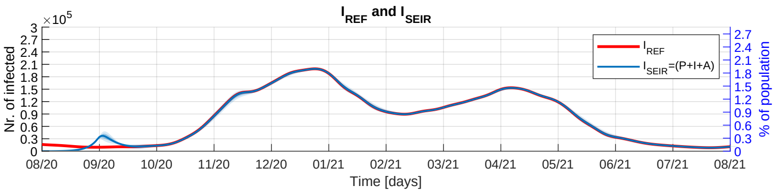


Figure 3: Required intervention stringency (top) and optimal test scheduling strategy (bottom) for respecting healthcare capacity in case of vaccines with different efficiency. The intervention cost (top) and test usage (percentage, bottom) can be seen in parentheses after each label.

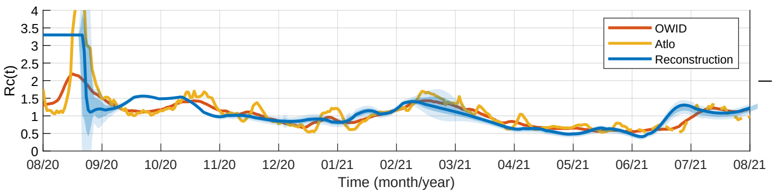
3.2 Robust trajectory reconstruction

We used both stochastic MPC and robust feedback-linearization (FDBL) with asymptotic output tracking for the trajectory reconstruction of different epidemic models. By transforming the estimation into a control problem, our method relies solely on the number of hospitalized individuals, updated daily in most countries. Nevertheless, even these values contained non-negligible inaccuracies (resulting from the caveats of administrative procedures) and required considerable preprocessing (moving average, spline interpolation, etc) to satisfy differentiability requirements. Adding an extra integrator term into the transformed system (sec. 2.3, eq. 5), effectively incrementing the relative degree ρ by one, increases the robustness of the FDBL to model- and parameter mismatch. To illustrate this robustness, we used different models for *control design* and *simulation*. For more realistic studies, we applied an extended Kalman filter (EKF) to compute some of the simulation model's states from the number of hospitalizations, and used only the estimated values for feedback. We carried out multiple simulations, altering the parameters on a grid of 10%–300%, monitoring the stability region and the deviance of the setup.

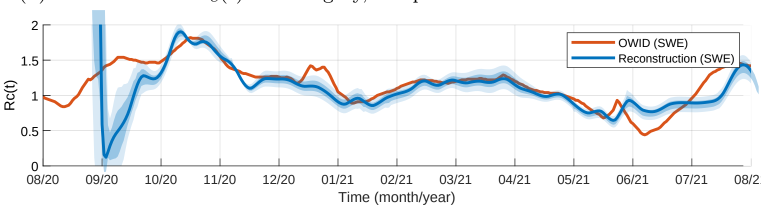
Figure 4a. shows the reference signal and actual, simulated output of Control setup 0. (mismatched parameters, but assuming perfect knowledge of the *simulation* model's states). After an initial transient period, the asymptotic output tracking produced barely observable errors, and the



(a) Tracking accuracy (mean and 2σ) with model mismatch, without EKF



(b) Reconstructed $R_c(t)$ for Hungary, compared to other results from literature



(c) Reconstructed $R_c(t)$ for Sweden, compared to other results from literature

Figure 4: Reference tracking and reconstruction capabilities of the robust controller

controller remained stable even for high parameter deviances.

Figures 4. also illustrates the estimated time-dependent reproduction number (sec. 2.1, eq. 1) for Hungary (4b) and Sweden (4c). Resulting from Control setup II. experiments (with EKF for the mismatched simulation model), the calculated input has higher deviance, but provides a more realistic reconstruction of the epidemic's spread after the initial transient. For reference, the figures also show reconstructions from independent literature, while the thesis compares the two countries' strategies as well.

3.3 Parameter synthesis of nonnegative systems

In this task, we try to find the parameters providing the desired qualitative dynamical properties by creating an appropriate nonlinear optimization problem and including the parameters as decision variables. Motivated by MPC (sec. 2.2), along with the parameters, we treat all future states of the time-discretized system up to a predefined finite horizon of M steps as decision variables, and introduce the system dynamics in the form of constraints. We also describe the desired behavior using appropriate constraints on the state variables (and manipulable inputs, if there are any). To prescribe oscillations, we can simply specify that the trajectories should periodically go above and below a threshold freely chosen by the controller (bounded decision variable). This kind of constraint can be easily expressed using the combination of the *always* and *eventually* STL operators, or even manually, as shown in the thesis. As in MPC, the objective function is usable to choose a preferred solution. In this case, however, it is sufficient to find any feasible solution.

The thesis presents three case studies. Figure 5. shows a time-invariant (fixed parameters, no seasonality) SEIR(S) epidemic model with waning immunity, capable of showing damped oscillations. Our solution can synthesize the right parameters for a desired frequency and amplitude.

In Figure 6. a three-species Lotka-Volterra food chain model can be observed. The parameters computed result in predefined approximate frequency and emergence/decay/sustentation of the chosen species.

The thesis also includes a Brussellator model for validation.

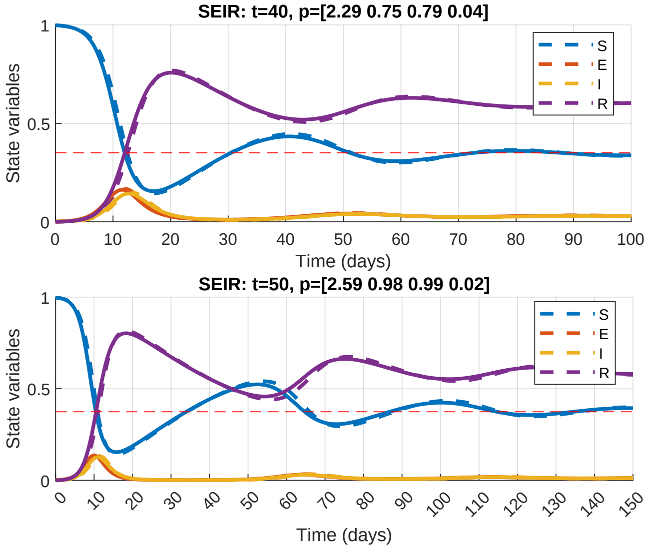


Figure 5: The SEIR(S) epidemic model's planned (dashed lines) and actual (solid) trajectories. The prescribed period and the obtained parameters are shown in the title.

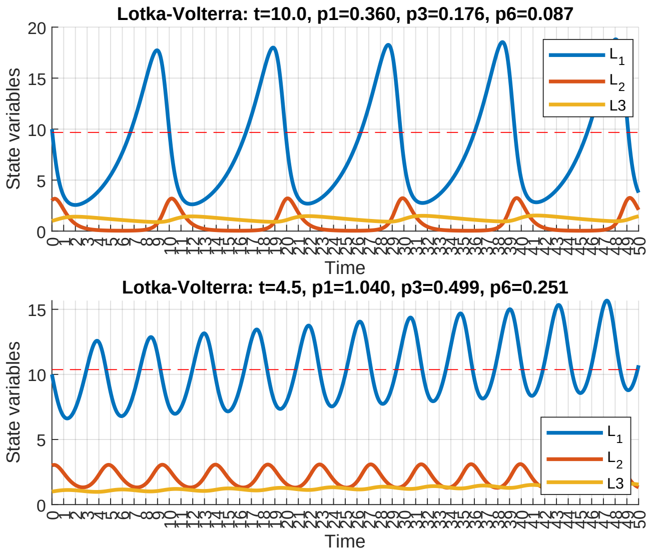


Figure 6: Computed parameters and corresponding trajectories for the Lotka-Volterra model. The red dashed line shows the chosen oscillation threshold for the L_1 species.

4 New scientific contributions

Thesis 1. I have presented a model predictive control-based methodology for the optimal control of nonlinear compartmental epidemic models allowing discrete intervention levels and intervals, in the presence of complex constraints specified by temporal logic formulas.

Thesis 1.1 I developed a method based on nonlinear model predictive control to compute the required stringency of epidemiological restrictions, ensuring the fulfillment of complex, time-varying and logical conditions, while balancing between possibly contradictory goals and expectations. The method is capable of handling predefined discrete intervention levels and time intervals.

Publication: [J1]

Thesis 1.2 I proposed a control theoretic approach for the integrated design of non-pharmaceutical interventions, vaccination and testing intensity for epidemic mitigation, introducing additional manipulable inputs and compartments to complex epidemic models. By accounting for the limited number of resources and the complex logical constraints, the optimization-based controller is capable of computing a comprehensive strategy for the timely deployment of the different measures.

Publication: [J2]

Related chapters: 3 (thesis), 3.1 (thesis booklet)

Thesis 2. I have designed novel methods for the retrospective trajectory reconstruction and parameter synthesis of nonlinear nonnegative systems, constructing and solving complex optimization problems inspired by the structure of deterministic or stochastic model predictive control.

Thesis 2.1 I have proposed optimization-based deterministic and stochastic methods for estimating the unmeasurable quantities of epidemic processes, together with error estimations. Using these, I gave precise approximations for the time-dependent

transmission rate, the likely actual number of infections, and the number of latent, pre-symptomatic, and asymptomatic cases based solely on the daily number of hospitalizations.
Publications: [C1], [J3]
Related chapters: 4.1 (thesis), 3.2 (thesis booklet)

Thesis 2.2 I have proposed a novel optimization-based parameter synthesis method, suitable to ensure a predefined qualitative behavior in nonlinear nonnegative systems. I have illustrated the methodology on three kinetic models, with the goal of inducing sustained or damped autonomous oscillatory behavior with given frequencies.
Publication: [J4]
Related chapters: 5 (thesis), 3.3 (thesis booklet)

Thesis 3. I have developed a robust, computationally efficient approach for historical data reconstruction of epidemic processes, using a robustified feedback-linearization based asymptotic reference tracking scheme together with nonlinear state estimation. The resulting setup showed appropriate robustness with respect to mismatch and inaccuracies in model structure, estimated model parameters, and measured output.
Publications: [C2], [C3], [C4], [C5], [J5]
Related chapters: 4.2 (thesis), 3.2 (thesis booklet)

5 Applications and future work

Due to the fact that we have developed new methodologies for a wide class of nonnegative systems, there are numerous application possibilities. Actually, some of the presented approaches were already applied in practice to address real-world data reconstruction needs.

During the COVID-19 pandemic, we used the presented framework to regularly estimate the number of individuals in unmeasurable categories (e.g. asymptomatic infections) in Hungary, providing insight into the progress of the current epidemic wave. Using these, we also computed accurate forecasts. Our results were always comparable (and sometimes even better) than the data published by independent research groups (e.g. [11, 12]).

The research concerning the robustification of the feedback-linearization technique to tolerate high model and parameter mismatch directly paved the way for the combination of compartmental-model-based control and agent-based modeling and simulation [13]. Being directly applicable in an upcoming epidemic (naturally, after tailoring the parameters to the spread and behavior of the potential new pathogen), the solution can be used to evaluate and balance between real-world epidemic control goals and intervention possibilities in rapidly changing environments.

Finally, as chemical oscillators play a fundamental role in numerous biological processes (e. g. circadian clock or other time-dependent cell decisions in living organisms), the possibility to synthesize such systems with predefined frequency and behavior might be helpful or thought-provoking in a wide area of biological and medical research.

There are several interesting directions left for future exploration:

1. The connection between the ODE and agent-based model could be made more realistic by optimally matching the combination of real-world interventions (e.g. school closure) to the intended strictness. Moreover, the ODE-based methodologies with multiple inputs (e.g. testing intensity, vaccination, etc) could also be complemented with agent-based approaches for optimized planning of an even more comprehensive epidemic management strategy.

2. Epidemic management aside, this kind of connection between robust controllers and agent-based models could provide a computationally feasible planning solution for all kinds of mechanical or ecological systems (population dynamics, vehicle traffic flows, etc.) Without connection to the epidemic management, preliminary studies were already carried out for optimized vehicle scheduling and route-planning in industrial environments using MPC and temporal logic [O1], [O2].

3. As kinetic models can be used to describe a wide range of processes, the application of the parameter synthesis methodology for e.g. ribosome flow models, calls for further investigation.

The Author's publications

The Author's journal papers

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